4,4-DIMETHYL-2-CYCLOPENTEN-1-ONE

Inchi: InChI=1S/C7H10O/c1-7(2)4-3-6(8)5-7/h3-4H,5H2,1-2H3
InchiKey: YVFVCSCZJJGBAK-UHFFFAOYSA-N
Formula: C7H10O
SMILES: CC1(C)C=CC(=O)C1
Mol. weight [g/mol]: 110.16

Physical Properties

Property code	Value	Unit	Source
hfus	2.25	kJ/mol	Joback Method
ie	9.55	eV	Cheméo Relay (1.0)
logp	1.542		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
ripol	1511.00		NIST Webbook
tb	431.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	191.44	J/mol×K	442.06	Joback Method
cpg	205.04	J/mol×K	479.92	Joback Method
cpg	217.69	J/mol×K	517.79	Joback Method
cpg	229.51	J/mol×K	555.65	Joback Method
cpg	240.59	J/mol×K	593.51	Joback Method
cpg	251.02	J/mol×K	631.37	Joback Method
cpg	260.90	J/mol×K	669.24	Joback Method

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22748169&Units=SI

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature